Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and Suisun Marsh

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Chapter 7: Implementation of a New DOC Growth Algorithm in DSM2-QUAL

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7 Implementation of a New DOC Growth Algorithm in DSM2-QUAL

7.1 Introduction

As part of DWR's Integrated Storage Investigations' In-Delta Storage project (ISI-IDS), DSM2-QUAL was modified to account for increases in dissolved organic carbon (DOC) concentrations due to the prolonged water contact with the peat soil on the proposed island reservoirs. The DWR Municipal Water Quality Investigations (MWQI) Program conducted the initial field experiments at DWR's SMARTS (Special Multipurpose Research and Technology Station) facility to develop the DOC growth algorithm to be used in QUAL (Pandey, 2002). Between 1998 and 2000, these experiments focused on measuring the production of DOC from peat soils in a series of eight tanks with different combinations of peat soil depth, water depth, and water exchange rates (Jung, 2001). However, while the SMARTS tank experiments did account for increases in DOC due to leaching and microbial decay, the experiments did not account for the additional production of organic carbon from algae and wetland plants. ISI conducted new studies that accounted for the production of organic carbon from algae and wetland plants in addition to the growth of DOC mass due to leaching and microbial decay of the peat soils (DuVall, 2003). This chapter summarizes the new methodology used in QUAL to simulate the increase in DOC mass in reservoirs due to interactions between water stored on a flooded Delta island and an island reservoir's peat soil bottom.

7.2 Implementation in QUAL

Based on the original SMARTS tank experiments (Jung, 2001), the concentration of DOC in the island reservoirs was modeled in QUAL using a logistic equation. Using this equation, island reservoir DOC would approach a fixed concentration after only a few months of storage. Since the implementation of this early equation, a few problems with this approach have been identified. First, the limited data from the SMARTS tank experiments suggested that after a few months, the DOC concentration in an island reservoir would approach a fixed value. However, the SMARTS tank experiments did not account for the production of organic carbon from algae and wetland plants, thus QUAL was underestimating the DOC concentration in the reservoirs. In situations where the DOC concentration of the diversions into one of the island reservoirs was higher than this fixed DOC concentration, QUAL would still use the logistic equation. In these situations the logistic equation would reduce the DOC concentration in the reservoir until it met the fixed DOC concentration.

In response to comments about the original SMARTS tank experiments and the implementation of the SMARTS data in QUAL, ISI conducted new experiments to develop stronger relationships from the new data (DuVall, 2003). These new studies accounted for the production of organic carbon from algae and wetland plants. Based on DuVall's work, the implementation of increasing DOC concentration in island reservoirs was completely redesigned in QUAL.

7.2.1 Activating DOC Growth

A new true / false flag, `storage_reservoir`, in the scalar.inp file (see Figure 7.1) allows anybody using the new QUAL executable to turn on / off the non-conservative growth of DOC in reservoirs. When the `storage_reservoir` flag is set to true, QUAL will look for a file called operation_schedule.dat in the directory were the QUAL run was initiated. In this file, constant monthly growth rates are specified only for the reservoirs where the user wants DOC concentrations to increase. When the `storage_reservoir` flag is set to false, DOC will be treated as a conservative constituent. DOC growth is limited to reservoirs.

```
# DSM2 input file
# ISI In-Delta Storage 2003 16-Year Planning Study
# Alternative B
# Updated: 2003.06.21, mmierzwa

# Various single-argument options (constants, coefficients, ...)
SCALAR
flush_output           10day          # interval to flush output
display_intvl          1day           # how often to display model time progress
checkdata              false          # check input data w/o simulation

# Note: all cont_* scalars are "true" or "false".
cont_unchecked         true           # continue on unchecked data
                                      # (use data value)
cont_question          false          # continue on questionable data
                                      # (use data value)
cont_missing           false          # continue on missing data
                                      # (use previous value)
cont_bad               false          # continue on bad data (use previous value)

warn_unchecked         false          # warn about unchecked data
warn_question          true           # warn about questionable data
warn_missing           false          # warn about missing data

printlevel             1                                 g, 0 to 9,
                                                         umber.

temp_dir               e:/trash

# following all QUAL variables
Qual_time_step         15min          # Qual time step, in minutes
Dispersion             t              # true Activate dispersion
Init_Conc              0.0            # initial concentration value (not used)
storage_reservoir      t              # storage Reservoirs
tide_length            25hour         # tide length
END
```

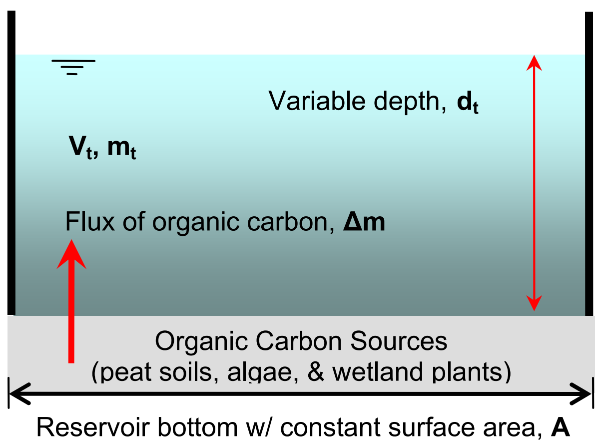
Flag to activate
(when set to true)
DOC growth

Figure 7.1: Sample scalar.inp File.

7.2.2 DOC Mass Growth Rate Parameters

The data from the new ISI tank studies did not suggest the same leveling off of the DOC concentration after a few months of storage that was observed in the original SMARTS data. Instead, DuVall noted a steady linear increase in DOC concentration that began in the spring and ended in the early fall. QUAL now uses monthly growth rates for each reservoir. The monthly growth rate for each reservoir can be changed to reflect data collected from different sites.

In the previous implementation (Pandey, 2002), the DOC equation directly calculated increases in the DOC concentration. In the case of the ISI-IDS project, the additional organic carbon in the reservoirs comes from either the peat soil bottom surface or the algae and wetland plants growing in the reservoir itself; thus QUAL's new growth mechanisms focus on adding organic carbon mass instead of DOC concentration. Because DSM2 treats reservoirs as tanks with constant surface areas, A, and variable depths, d_t, the amount of organic carbon added to the stored water, Δm, is a linear function of surface area (Figure 7.2). Though the new organic carbon, Δm, is shown below as coming from the peat soil base, the monthly growth rate is based on field observations that also included algae and plant sources. The new DOC concentration, C_t, will be calculated each time step using the current reservoir volume (except when the reservoir is below a specified depth, as described below), V_t, and the total mass of organic carbon, m_t', which includes both the mass already present in the reservoir, m_t, and new mass added to the system, Δm.



$$V_t = d_t \cdot A$$

$$m_t' = m_t + \Delta m$$

$$C_t = m_t' / V_t$$

Figure 7.2: Conceptualization of Implementation of DOC Growth in QUAL.

Even though the flux of organic carbon is a constant value, the concentration may grow at a non-linear rate when the volume of the reservoir is changing. This can become problematic in situations when water is being released from a reservoir because the decreasing volume and constant flux of organic carbon into the reservoir will increase the rate of growth of the DOC concentration. An increase in the rate of DOC growth becomes a numerical problem as the volume of the reservoir approaches zero.

To prevent this, a minimum reservoir depth limit is specified in the operation_schedule.dat file (Figure 7.3). When the stage in a reservoir is equal to or less than this limit, QUAL no longer calculates a change in the DOC concentration in the reservoir.

The amount of new organic carbon is calculated as a function of the surface area of the reservoir, from QUAL's reservoirs.inp file, and the monthly growth rate parameters from the operation_schedule.dat file (see Figure 7.3). The monthly growth rate coefficients start in October and continue through the rest of the water year. The next parameter in the operation_schedule.dat file is a scaling factor. QUAL simulates DOC in ug/L, so the scaling factor is used to adjust the monthly growth rates accordingly. For the example operation_schedule.dat file shown below, the scaling favor is 1000.0. The final growth parameter is the minimum depth for growth limit described above.

```
Description of Input Variables
Line 1 Total Number of Reservoirs used for Storage Purposes
Line 2 Name of the Storage Reservoir followed by DOC Growth Parameters
Lines 2 should be repeated for each reservoir
2
webbtract     0.47 0.0 0.0 0.0 0.0 0.47 0.47 0.47 0.47 0.47 0.47 0.47 1000.0 2.0
baconisland   0.47 0.0 0.0 0.0 0.0 0.47 0.47 0.47 0.47 0.47 0.47 0.47 1000.0 2.0
```

Organic Carbon Monthly Growth Rate | Scaling Factor | Min. Depth for Growth

Figure 7.3: Example operation_schedule.dat File.

7.3 Example Application of New Methodology

This new method of DOC growth was tested in QUAL using the growth rate parameters shown in Figure 7.3, with the exception that the October growth rate constant was specified as 0.0 instead of 0.47. The hydrology and operation of the reservoirs were identical to a previous DSM2 study that used the old DOC growth logistic equation. The previous equation approach made use of different "bookends" for estimating the DOC growth parameters. Typically two bookends would be chosen to represent a high ultimate DOC concentration and a low ultimate DOC concentration. Finally, using the `storage_reservoir` flag shown in Figure 7.1, DOC growth was turned off to represent a no-growth base case.

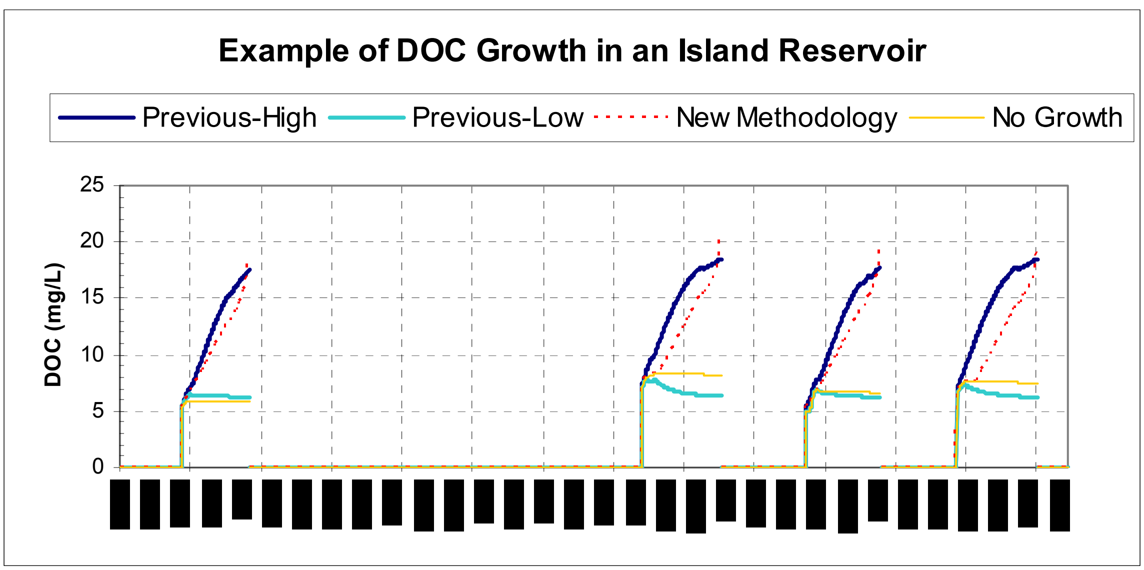


Figure 7.4: Example of DOC Growth in an Island Reservoir.

A comparison of the DOC concentrations from the previous equation high and low bookends, this new methodology, and a no-growth base case in an island reservoir is shown in Figure 7.4. DOC is shown only at times when the stage in the reservoir was greater than 1.0 ft. As can be seen by the no-growth results, the initial DOC concentration in the reservoir is a function of the diversions from nearby channels and varied over the course of the study. Reservoir releases have no impact on the concentration inside the reservoirs.

During many of the diversion (fill) periods, the ultimate DOC concentration for the low bookend derived from the previous equation was lower than the incoming DOC concentration. Thus when the initial DOC concentration was greater than 6 mg/L, the low bookend equation reduced the DOC concentration in the reservoir. As described above, this problem is one of the reasons the DOC growth implementation in QUAL was redesigned.

The DOC concentration for the previous high bookend and the new methodology reached similar maximum values by the end of the four to five month storage periods. However, the DOC concentrations for the new methodology tended to have a sharp increase during the release period. As was described above in section 7.2.2, when the volume of the reservoir decreases, but the growth rate remains constant, the rate of change of the actual DOC concentration will rapidly increase. It is for this reason that a minimum depth required for growth limit is specified with the new DOC growth rate parameters. For this example, the minimum depth for DOC growth was set at 2 ft.

Although the previous high bookend and new methodology results were similar for this example, if the storage period was longer, the DOC concentration in the new methodology would continue to increase over time, while the DOC concentration using the previous high bookend method would quickly approach its ultimate DOC concentration (which for this example was around 19 mg/L). The difference between these two methodologies lies in the conclusions drawn from the field experiments. Because DuVall's field investigations were extended beyond the length of the original experiments, the new methodology is more effective at simulating the impacts of potential carry-over storage events (i.e., long-term storage).

7.4 Conclusions

By comparing the results of the new DOC growth implementation with the results of the previous implementation and no-growth studies, it has been confirmed that the actual implementation of the new DOC methodology in QUAL produces reasonable results, while avoiding some of the problems associated with the previous implementation. Though the above example only shows the DOC concentration at times when there is significant storage in the reservoirs (i.e., the stage is greater than 1 ft.), the proper indexing of the monthly growth rates was confirmed by looking at the DOC concentration of the new implementation for an entire six-year period.

However, it is important to note that although the implementation of the new DOC growth methodology in QUAL performed adequately when tested using a prior ISI-IDS study operation, the following points should be considered when using the new methodology:

- Non-conservative DOC growth is currently only available in QUAL for reservoirs. This non-conservative growth may be activated for specific reservoirs, while other constituents will be unaffected by the DOC growth parameters.

- A special QUAL executable was created for DOC growth. While this executable has been tested for DOC and other conservative constituents, it is not being distributed (i.e., it is only available upon request). Furthermore, the new `storage_reservoir` flag added to the scalar.inp file cannot be read in an older version of QUAL.

- The growth rate parameters are site specific. When using this version of QUAL to simulate DOC growth, the growth rate parameters should be valid for the reservoir to which they are applied.

7.5 References

DuVall, R. (2003). "In-Delta Storage Program Water Quality Field Investigations". Presentation on Jan. 22, 2003 to stakeholders committee meeting. Available at http://www.isi.water.ca.gov/ssi/indelta/docs/4%20FieldInvStakeholders012203.ppt. Sacramento, CA.

Jung, M. (2001). *Conceptual Model and Mathematical Relationships for Reservoir Island Release Water Quality Module in DSM2 for Organic Carbon*. Consultant's Report. Municipal Water Quality Investigations, California Department of Water Resources. Sacramento, CA.

Pandey, G. (2002). "Chapter 9: Implementation of DOC Growth in DSM2-QUAL." *Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and Suisun Marsh. 23rd Annual Progress Report to the State Water Resources Control Board*. California Department of Water Resources. Sacramento, CA.